WELCOME !

Workshop Organizers: **Mark Hybertsen, CFN, BNL**
Ping Liu, CFN & Chemistry, BNL
Deyu Lu, CFN, BNL
Artem Oganov, SBU

Hands-on with VASP: **VASP Team**
Martijn Marsman, U. Vienna

Workshop Coordinator: **Denean McArthur, CFN, BNL**

A joint workshop of the Center for Functional Nanomaterials at Brookhaven National Laboratory
and the Center for Materials by Design at Stony Brook University,
with support from a SBU-BNL Seed grant

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Safety First: In an Emergency . . .

Fire Alarms at the CFN

There are **two** distinctly different alarm rings at the CFN.

Click icons to hear alarms

1. The normal fire alarm ring - which will ring if a fire is detected.

   Exit the building by the nearest exit and go to the outdoor assembly area in the west parking lot.

2. The second fire alarm is called a **Temporal 3 Alarm** - it sounds three bongs followed by this message on the PA system: "*Hazardous gas release, Exit from the north (front) side of the building only.*" Go to the outdoor assembly area in the west parking lot, unless otherwise directed.

CFN = Evacuation Zone 10

Nota bene: Regular alarm test Mondays at noon

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Assembly Areas

Indoor Assembly Area

Located in the center corridor of the CFN towards the rear doors

Indoor: Back of Lobby

Outdoor: Parking Lot

Outdoor Assembly Area

Located in the west parking lot by the curved concrete wall

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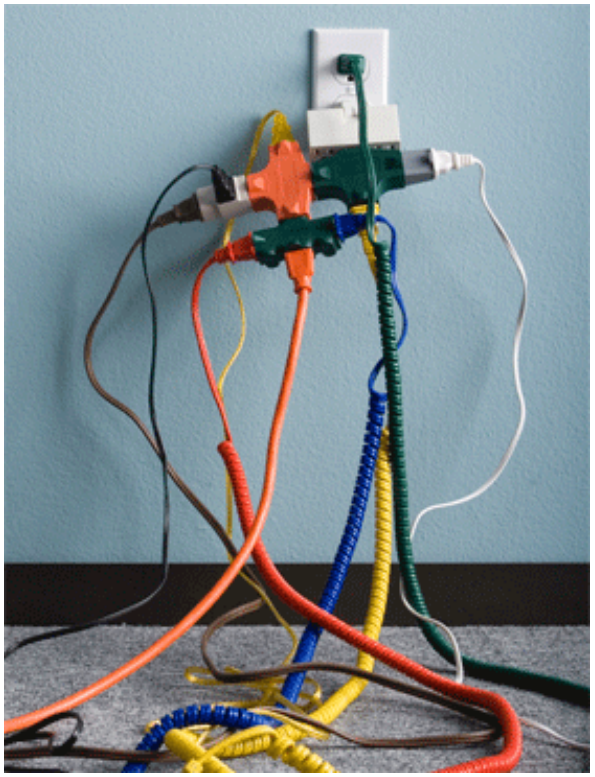
Safety First: A Note Regarding Electrical Cords



Please use outlets in the tables or the power strips provided.

Ask if you need help with power access.

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The Center for Functional Nanomaterials: A User-Oriented Nanoscience Research Facility

One of five DOE funded Nanoscience User Facilities

Mission

- Enable user-driven nanoscience
- Conduct research in energy-related nanomaterials

Thematic and cross-cutting groups

- electronic nanomaterials
- interface science and catalysis
- soft and biomaterials

theory & computation

electron microscopy

CREATE	CHARACTERIZE		UNDERSTAND
Materials Synthesis	Proximal Probes	X-ray Probes	Data Management
Nanofabrication	Electron Microscopy	UV Probes	Theory & Simulation
Self-Assembly	Optical Spectroscopy	NSLS-II Stations	Computer Facility

Block-copolymer | E-beam Lithography | Reactor STM | AC ETEM | AC LEEM | AP XPS | Theory

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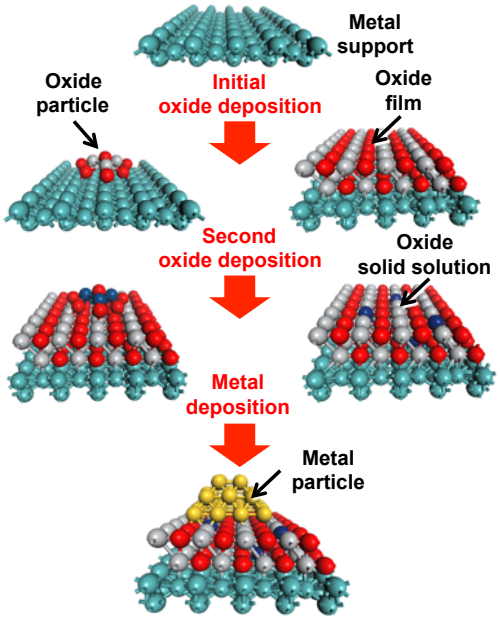
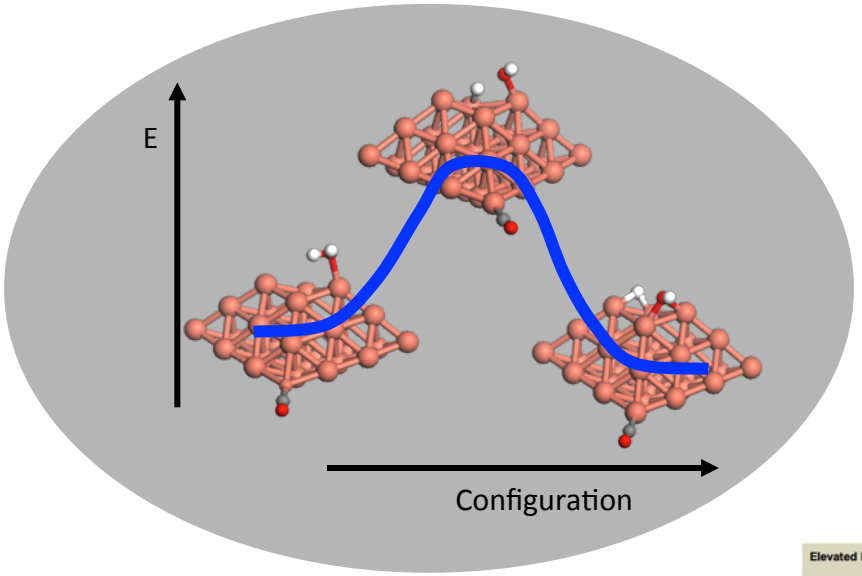
Theory: Fitting the Puzzle Together

Synthesis & Assembly of Nanomaterials



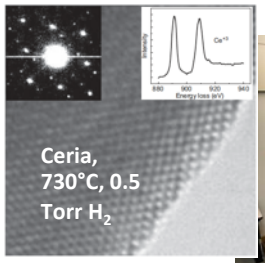
Development of Catalytic Functionality

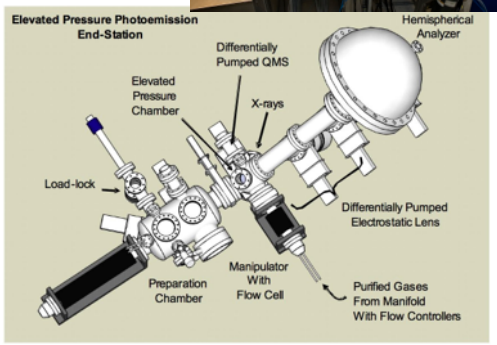
Microscopic Models: Structure & Function



Shared goal: Staff & Users

In situ & *operando* Characterization Techniques





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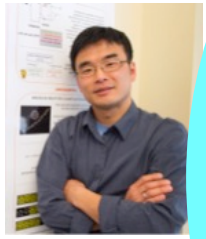
Theory Group

Mark Hybertsen
Electronic & optical properties of nanostructures

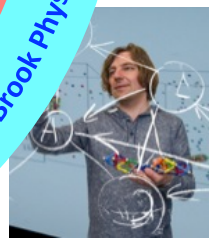
Ping Liu
Structure & activity: heterogeneous catalysis (CFN 25%)

Qin Wu
Quantum chemistry & organic materials

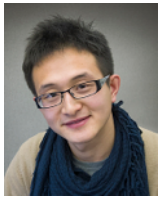


Deyu Lu
Electronic structure theory & interface science

Alexei Tkachenko
Soft matter theory & directed assembly



Post-doctorals



Xiaochuan Ge

Jack Lyons

Externally funded:

Neerav Kharche, Post-doc, CMCSN (DOE)
Adrian Soto, PhD student, BNL-SBU seed

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Theory & Computation Facility

Staff Expertise

- Phenomena, theory & method development
- Support for widely used packages

Vibrant User Community

- Research topics strongly overlap to CFN thematic emphasis
- Experiment-theory collaboration

One third of open user projects include staff collaboration

Computer

Hardware:

Aggregate > 2100 cores
Infiniband networks
Supporting storage

Software & Packages:

VASP, QE, Gaussian, …
LAMMPS, Reactive MD, …

BNL ITD machine room & system admin.

Resource Allocation:

60% Peer reviewed users
(12 million core-hrs, F2013)

15% Internal research
15% Facility development

10% Downtime, friction, …

(Relative to 24x7)

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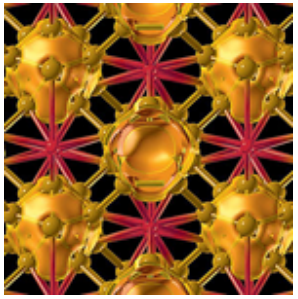
Center for Materials by Design

Artem Oganov, Geosciences & Physics Depts. Stony Brook University

CFN User

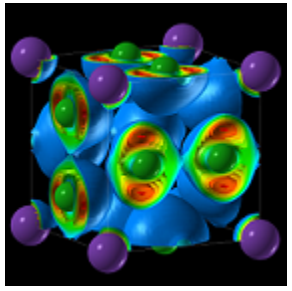
Pioneer in evolutionary algorithms for materials discovery:
USPEX code

New super-hard and ionic phase of boron



Oganov, et al., Nature 457, 863, 2009

Unexpected phases in the sodium chloride family: Na_3Cl, Na_2Cl, Na_3Cl_3, $NaCl_3$, $NaCl_7$



Zhang, et al., Science 342, 1502, 2013

Our Workshop: Focus on Interface Science & Catalysis

Joint training and outreach:
CFN staff and user community

Current developments & opportunities in research, including impact of experiment-theory collaboration

Introduction to theory & computational approaches, from fundamentals to applications

Tutorials and practical exercises with VASP, one of the widely used suites of computational tools in this field.
Supported by the VASP Team: Martijn Marsman, U. Vienna

Opportunity: Discuss future research & user projects with CFN staff.

Wednesday afternoon: Open discussion time by design – send us requests

Practical Matters

All guests need to have registered at the GUV center (Bldg 400)

- If not done yet, please do it today at lunch time

Registered attendees: Meal tickets

- Breakfast and breaks here
- Lunch at Berkner Hall: General seating
- Dinners at Berkner Hall Monday, Tuesday & Thursday
- Wednesday dinner at the Riverhead Aquarium (transportation provided)

Tutorials and Computational Exercises

- Access to CFN cluster required, using your lap-top as a portal
- Main visualization software: P4Vasp
- Support for remaining technical problems at 10:00 and again at 1:00, here

Group photo on Wednesday at 3:00 PM

Program for Today

Monday, November 3, 2014

08:15 - 08:29	Breakfast *14'*
08:29 - 08:30	Fundamentals of Electronic Structure of Materials and Density Functional Theory *Overview of materials challenges in the energy arena. Introduction to essential methodologies used to compute the properties of materials, including basics of DFT methodologies.*
08:30 - 09:15	Welcome & Overview, Mark Hybertsen, BNL *45'*
09:15 - 10:00	Energy Materials Challenges, Cynthia Friend, Harvard *45'*
10:00 - 10:30	Break
10:30 - 11:15	Introduction to Pseudopotentials and Electronic Structure, Phil Allen, Stony Brook University *45'*
11:15 - 12:00	Introduction to Density Functional Theory, Deyu Lu, BNL *45'*
12:00 - 13:30	Lunch -- Berkner *1h30'*
13:30 - 15:00	Tutorial 1: Intro to Vasp Calculations for Solids, Martijn Marsman, U.Wien *1h30'*
15:00 - 15:30	Break
15:30 - 17:00	Tutorial 2: Intro to Vasp Calculations for Surfaces, Martijn Marsman, U. Wien *1h30'*
18:00	Dinner -- Berkner *1h30'*